checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: I

```
Bond precision:    Al- O = 0.0144 A           Wavelength=0.02510

Cell:              a=8.688(3)       b=5.024(2)            c=9.734(4)
                   alpha=90         beta=90.77(2)         gamma=90
Temperature:       293 K

                   Calculated                 Reported
Volume             424.8(3)                   424.9(3)
Space group        P 21/n                     P 1 21/n 1
Hall group         -P 2yn                     -P 2yabc
Moiety formula     Al2 F H5 O5                ?
Sum formula        Al2 F H5 O5                Al2 F1 H5 O5
Mr                 158.00                     158.00
Dx,g cm-3          2.470                      2.470
Z                  4                          4
Mu (mm-1)          0.000                      0.000
F000               0.0                        104.6
F000'              319.93
h,k,lmax                                      11,7,13
Nref                                          2672
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness=                  Theta(max)= 1.010

R(reflections)= 0.1524( 2141)                 wR2(reflections)=
                                              0.3171( 2672)
S = 7.151                  Npar= 42
```

The following ALERTS were generated. Each ALERT has the format
        test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

ATOM007_ALERT_1_A _atom_site_aniso_label is missing
            Unique label identifying the atom site.

Author Response: All atoms were refined with one isotropic displacement parameter.

DIFMN02_ALERT_2_A The minimum difference density is < -0.1*ZMAX*2.00
            _refine_diff_density_min given =   -5.550
            Test value =   -2.600

Author Response: Ripples in the difference density map appear as a consequence of not fully modeled dynamical effects and structure disorder.

GOODF01_ALERT_2_A The least squares goodness of fit parameter lies
            outside the range 0.40 <> 6.00
            Goodness of fit given =   7.151

Author Response: GooF parameters is not reliable for dynamical refinement of electron diffraction data.

PLAT087_ALERT_2_A Unsatisfactory S value (Too High) ....   7.15 Check

Author Response: GooF parameters is not reliable for dynamical refinement of electron diffraction data.

PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value ....   Please Do !

Author Response: Cell parameters were determined by the software PETS. No output information for this parameter was given.

PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ......   Please Do !

Author Response: Cell parameters were determined by the software PETS. No output information for this parameter was given.

PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ......   Please Do !

Author Response: Cell parameters were determined by the software PETS. No output information for this parameter was given.

```
PLAT355_ALERT_3_A Long    O-H (X0.82,N0.98A)  O6       - H6      .      1.14 Ang.
```

Author Response: O-H distances determined by electron diffraction are generally longer than the same determined by X-rays.

```
PLAT881_ALERT_1_A No Datum for _diffrn_reflns_av_R_equivalents ...    Please Do !
```

Author Response: Data were refined dynamically considering separetely each electron diffraction pattern.

🟠 Alert level B
```
PLAT355_ALERT_3_B Long    O-H (X0.82,N0.98A)  O1       - H1      .      1.08 Ang.
```

Author Response: O-H distances determined by electron diffraction are generally longer than the same determined by X-rays.

```
PLAT355_ALERT_3_B Long    O-H (X0.82,N0.98A)  O3       - H3      .      1.12 Ang.
```

Author Response: O-H distances determined by electron diffraction are generally longer than the same determined by X-rays.

```
PLAT416_ALERT_2_B Short Intra D-H..H-D        H1      ..H6       .      1.46 Ang.
                                              x,y,z  =     1_555 Check
```

Author Response: H1 and H6 positions could not be properly refined; inaccuracies in fractional coordiantes are possible.

🟡 Alert level C
```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings  Differ    Please Check
             Calc: Al2 F H5 O5
             Rep.: Al2 F1 H5 O5
PLAT082_ALERT_2_C High R1 Value ..................................    0.15 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................    0.32 Report
PLAT127_ALERT_1_C Implicit Hall Symbol  Inconsistent with Explicit   -P 2yabc Check
PLAT355_ALERT_3_C Long    O-H (X0.82,N0.98A)  O5       - H5      .      1.05 Ang.
```

Author Response: O-H distances determined by electron diffraction are generally longer than the same determined by X-rays.

```
PLAT417_ALERT_2_C Short Inter D-H..H-D        H1       ..H3      .        2.11 Ang.
                                      1/2-x,1/2+y,-1/2-z  =      2_554 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D        H1       ..H6      .        2.14 Ang.
                                        -x,2-y,-z  =      3_575 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D        H5       ..H6      .        2.10 Ang.
                                      1/2+x,3/2-y,1/2+z  =      4_565 Check
PLAT799_ALERT_4_C Numeric Label on Displacement Par. Record ......        ? Check
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension       2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF    Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)     293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)     293 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)    .     2.72 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)    .     2.89 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       6 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of      3.0 Sig(I)
```

```
   9 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

  13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   5 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock I - ellipsoid plot